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# MOLSCAT: a program for non-reactive quantum scattering calculations on atomic and molecular collisions

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## Abstract

MOLSCAT is a general-purpose program for quantum-mechanical calculations on nonreactive atom-atom, atom-molecule and molecule-molecule collisions. It constructs the coupled-channel equations of atomic and molecular scattering theory, and solves them by propagating the wavefunction or log-derivative matrix outwards from short range to the asymptotic region at long range. It then applies scattering boundary conditions to extract the scattering matrix (S matrix). Built-in coupling cases include atom + rigid linear molecule, atom + vibrating diatom, atom + rigid symmetric top, atom + asymmetric or spherical top, rigid diatom + rigid diatom, rigid diatom + asymmetric top, and diffractive scattering of an atom from a crystal surface. Interaction potentials may be specified either in program input (for simple cases) or with user-supplied routines. For the built-in coupling cases, MOLSCAT can loop over total angular momentum (partial wave) and total parity to calculate elastic and inelastic integral cross sections and spectroscopic line-shape cross sections. Post-processors are available to calculate differential cross sections, transport, relaxation and Senftleben-Beenakker cross sections, and to fit the parameters of scattering resonances. MOLSCAT also provides an interface for plug-in routines to specify coupling cases (Hamiltonians and basis sets) that are not built in; plug-in routines are supplied to handle collisions of a pair of alkali-metal atoms with hyperfine structure in an applied magnetic field. For low-energy scattering, MOLSCAT can calculate scattering lengths and effective ranges and can locate and characterise scattering resonances as a function of an external variable such as the magnetic field.

**Keywords:** S matrix, cross section, elastic, inelastic, Feshbach resonance, external fields

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## PROGRAM SUMMARY

*Manuscript Title:* MOLSCAT: a program for non-reactive quantum scattering calculations on atomic and molecular collisions

*Authors:* Jeremy M. Hutson and C. Ruth Le Sueur

*Program Title:* MOLSCAT

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*Programming language:* Fortran 90

*Computer:*

*Operating system:*

*RAM:* case dependent

*Keywords:* S matrix, cross section, elastic, inelastic, Feshbach resonance, external fields

*Classification:* 16.7 Elastic Scattering and Energy Transfer

*External routines/libraries:* LAPACK, BLAS

*Subprograms used:*

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*Nature of problem:*

Quantum-mechanical calculations of scattering properties for non-reactive collisions between atoms and molecules.

*Solution method:*

The Schrödinger equation is expressed in terms of coupled equations in the interparticle distance,  $R$ . Solutions of the coupled-channel equations are propagated outwards from the classically forbidden region at short range to the asymptotic region. The program calculates scattering S matrices and uses them to calculate scattering properties including elastic, inelastic and line-shape cross sections.

*Unusual features:*

1. MOLSCAT contains numerous features to handle quantities important in low-energy collisions. It can propagate very efficiently to very long range, and it can calculate low-energy properties such as the scattering length (complex and energy-dependent if required) and the effective range.
2. MOLSCAT can construct and solve sets of coupled equations using basis sets that are not eigenfunctions of the Hamiltonians of the colliding particles at long range. The propagation is carried out in the primitive basis set, and the solutions are transformed to the asymptotic basis set before applying long-range boundary conditions to extract the S matrix.
3. MOLSCAT provides an interface that allows users to specify the coupled equations that arise from additional Hamiltonians and basis sets.
4. MOLSCAT provides an interface that allows users to include multiple external fields in the Hamiltonian. This same interface also allows users to include a factor which scales the interaction potential, and to investigate how properties vary with this factor.
5. MOLSCAT can locate and characterise low-energy Feshbach resonances either as a function of collision energy or as a function of external fields or of the potential scaling factor.

*Running time:* Highly dependent on mass and complexity of interacting particles

## 1. Introduction

MOLSCAT solves the quantum-mechanical non-reactive scattering problem for systems where the total Hamiltonian of the colliding pair may be written

$$H = -\frac{\hbar^2}{2\mu}R^{-1}\frac{d^2}{dR^2}R + \frac{\hbar^2\hat{L}^2}{2\mu R^2} + H_{\text{intl}}(\xi_{\text{intl}}) + V(R, \xi_{\text{intl}}), \quad (1)$$

where  $R$  is a radial coordinate describing the separation of two particles and  $\xi_{\text{intl}}$  represents all the other coordinates in the system.  $H_{\text{intl}}$  represents the sum of the internal Hamiltonians of the isolated particles, and depends on  $\xi_{\text{intl}}$  but not  $R$ , and  $V(R, \xi_{\text{intl}})$  is an interaction potential. The operator  $\hbar^2\hat{L}^2/2\mu R^2$  is the centrifugal term that describes the end-over-end rotational energy of the interacting pair.

Scattering problems of this type commonly arise in atomic and molecular collisions [1]. The observable quantities are often differential or integral cross sections for elastic and inelastic collisions processes, or the corresponding thermally averaged rate coefficients. There are also cross sections that describe relaxation properties and spectroscopic line shapes (line widths, line shifts and line mixing) [2] and transport properties and Senftleben-Beenakker effects [3]. Scattering calculations are also used to model spectroscopic line positions, widths and lifetimes for predissociating states of van der Waals complexes [4]. Somewhat different applications arise for ultracold atomic and molecular collisions [5], where the quantities of interest are often scattering lengths, total inelastic loss rates, and the properties of zero-energy Feshbach resonances.

The internal Hamiltonian  $H_{\text{intl}}$  is a sum of terms for the two particles 1 and 2,

$$H_{\text{intl}}(\xi_{\text{intl}}) = H_{\text{intl}}^{(1)}(\xi_{\text{intl}}^{(1)}) + H_{\text{intl}}^{(2)}(\xi_{\text{intl}}^{(2)}), \quad (2)$$

with eigenvalues  $E_{\text{intl},i} = E_{\text{intl},i}^{(1)} + E_{\text{intl},i}^{(2)}$ , where  $E_{\text{intl},i}^{(1)}$  and  $E_{\text{intl},i}^{(2)}$  are energies of the separated monomers 1 and 2. The individual terms can vary enormously in complexity: each one may represent a structureless

atom, requiring no internal Hamiltonian at all, a vibrating and/or rotating molecule, or a particle with electron and/or nuclear spins. The problems that arise in ultracold physics frequently involve pairs of atoms or molecules with electron and nuclear spins, often in the presence of external electric, magnetic or photon fields. All these complications can be taken into account in the structure of  $H_{\text{intl}}$  and the interaction potential  $V(R, \xi_{\text{intl}})$ , which may both involve terms dependent on spins and external fields.

MOLSCAT solves the Schrödinger equation for the Hamiltonian (1) using the *coupled-channel* approach, which handles the radial coordinate  $R$  by direct numerical propagation on a grid, and all the other coordinates using a basis set. In the coupled-channel approach, the total wavefunction is expanded

$$\Psi(R, \xi_{\text{intl}}) = R^{-1} \sum_j \Phi_j(\xi_{\text{intl}}) \psi_j(R), \quad (3)$$

where the functions  $\Phi_j(\xi_{\text{intl}})$  form a complete orthonormal basis set for motion in the coordinates  $\xi_{\text{intl}}$  and the factor  $R^{-1}$  serves to simplify the form of the radial kinetic energy operator. The wavefunction in each *channel*  $j$  is described by a radial *channel function*  $\psi_j(R)$ . The expansion (3) is substituted into the total Schrödinger equation, and the result is projected onto a basis function  $\Phi_i(\xi_{\text{intl}})$ . The resulting coupled differential equations for the channel functions  $\psi_i(R)$  are

$$\frac{d^2 \psi_i}{dR^2} = \sum_j [W_{ij}(R) - \mathcal{E} \delta_{ij}] \psi_j(R). \quad (4)$$

Here  $\delta_{ij}$  is the Kronecker delta and  $\mathcal{E} = 2\mu E/\hbar^2$ , where  $E$  is the total energy, and

$$W_{ij}(R) = \frac{2\mu}{\hbar^2} \int \Phi_i^*(\xi_{\text{intl}}) [\hbar^2 \hat{L}^2 / 2\mu R^2 + H_{\text{intl}} + V(R, \xi_{\text{intl}})] \Phi_j(\xi_{\text{intl}}) d\xi_{\text{intl}}. \quad (5)$$

The different equations are coupled by the off-diagonal terms  $W_{ij}(R)$  with  $i \neq j$ .

The coupled equations may be expressed in matrix notation,

$$\frac{d^2 \boldsymbol{\psi}}{dR^2} = [\mathbf{W}(R) - \mathcal{E} \mathbf{I}] \boldsymbol{\psi}(R). \quad (6)$$

If there are  $N$  basis functions included in the expansion (3),  $\boldsymbol{\psi}(R)$  is a column vector of order  $N$  with elements  $\psi_j(R)$ ,  $\mathbf{I}$  is the  $N \times N$  unit matrix, and  $\mathbf{W}(R)$  is an  $N \times N$  interaction matrix with elements  $W_{ij}(R)$ .

In general there are  $N$  linearly independent solution vectors  $\boldsymbol{\psi}(R)$  that satisfy the Schrödinger equation subject to the boundary condition that  $\boldsymbol{\psi}(R) \rightarrow 0$  in the classically forbidden region at short range. These  $N$  column vectors form a wavefunction matrix  $\boldsymbol{\Psi}(R)$ . The various propagators in MOLSCAT work either by propagating  $\boldsymbol{\Psi}(R)$  and its radial derivative  $\boldsymbol{\Psi}'(R)$  or by propagating the log-derivative matrix  $\mathbf{Y}(R) = \boldsymbol{\Psi}'(R)[\boldsymbol{\Psi}(R)]^{-1}$ .

The particular choice of the basis functions  $\Phi_j(\xi_{\text{intl}})$  and the resulting form of the interaction matrix elements  $W_{ij}(R)$  depend on the physical problem being considered. The complete set of coupled equations often factorises into blocks determined by the symmetry of the system. In the absence of external fields, the *total angular momentum*  $J_{\text{tot}}$  and the *total parity* are conserved quantities. Different or additional symmetries arise in different physical situations. MOLSCAT is designed to loop over total angular momentum and parity, constructing a separate set of coupled equations for each combination and solving them by propagation. These loops may be repurposed for other symmetries when appropriate.

MOLSCAT can also handle interactions that occur in external fields, where the total angular momentum is no longer a good quantum number.

### 1.1. Matrix of the interaction potential

In order to streamline the calculation of matrix elements for the propagation, MOLSCAT expresses the interaction potential in an expansion over the internal coordinates,

$$V(R, \xi_{\text{intl}}) = \sum_{\Lambda} v_{\Lambda}(R) \mathcal{V}^{\Lambda}(\xi_{\text{intl}}). \quad (7)$$

The specific form of the expansion depends on the nature of the colliding particles. The radial potential coefficients  $v_\Lambda(R)$  may either be supplied explicitly, or generated internally by numerically integrating over  $\xi_{\text{intl}}$ . The  $R$ -independent coupling matrices  $\mathbf{V}^\Lambda$  with elements  $\mathcal{V}_{ij}^\Lambda = \langle \Phi_i | \mathcal{V}^\Lambda | \Phi_j \rangle_{\text{intl}}$  are calculated once and stored for use in evaluating  $W_{ij}(R)$  throughout the course of a propagation.

### 1.2. Matrices of the internal and centrifugal Hamiltonians

Coupled-channel scattering theory is most commonly formulated in a basis set where  $\hat{L}^2$  and  $H_{\text{intl}}$  are both diagonal. All the built-in coupling cases use basis sets of this type. The matrix of  $H_{\text{intl}}$  is  $\langle \Phi_i | H_{\text{intl}} | \Phi_j \rangle_{\text{intl}} = E_{\text{intl},i} \delta_{ij}$ . The diagonal matrix elements of  $\hat{L}^2$  are often of the form  $L_i(L_i + 1)$ , where the integer quantum number  $L_i$  (sometimes called the partial-wave quantum number) represents the end-over-end angular momentum of the two particles about one another.

However, MOLSCAT also allow the use of basis sets where one or both of  $\hat{L}^2$  and  $H_{\text{intl}}$  are non-diagonal. If  $H_{\text{intl}}$  is non-diagonal, it is expanded as a sum of terms

$$H_{\text{intl}}(\xi_{\text{intl}}) = \sum_{\Omega} h_{\Omega} \mathcal{H}_{\text{intl}}^{\Omega}(\xi_{\text{intl}}), \quad (8)$$

where the  $h_{\Omega}$  are scalar quantities, some of which may represent external fields if desired. MOLSCAT generates additional coupling matrices  $\mathcal{H}^{\Omega}$  with elements  $\mathcal{H}_{ij}^{\Omega} = \langle \Phi_i | \mathcal{H}_{\text{intl}}^{\Omega} | \Phi_j \rangle_{\text{intl}}$ . These are also calculated once and stored for use in evaluating  $W_{ij}(R)$  throughout the course of a propagation. A similar mechanism is used for basis sets where  $\hat{L}^2$  is non-diagonal, with

$$\hat{L}^2 = \sum_{\Upsilon} \mathcal{L}^{\Upsilon}. \quad (9)$$

If  $H_{\text{intl}}$  is non-diagonal, the allowed energies  $E_{\text{intl},i}$  of the pair of monomers at infinite separation are the eigenvalues of  $H_{\text{intl}}$ . The wavefunctions of the separated pair are represented by simultaneous eigenvectors of  $H_{\text{intl}}$  and  $\hat{L}^2$ .

### 1.3. Boundary conditions at short range

For scattering calculations where the origin is energetically inaccessible, it is often sufficient to require that  $\Psi(R) \rightarrow 0$  in the classically forbidden region at short range, or equivalently that  $\mathbf{Y}(R) \rightarrow \pm\infty$ . However, it is usually more efficient to apply a boundary condition based on the Wentzel-Kramers-Brillouin (WKB) approximation,

$$Y(R) \approx k(R), \quad (10)$$

where  $k(R) = [2\mu(V(R) - E)/\hbar^2]^{1/2}$  and  $V(R)$  is an effective potential energy for the channel concerned. For locally closed channels, MOLSCAT applies the boundary conditions (10) by default. This gives faster convergence with respect to  $R_{\text{min}}$  than  $\mathbf{Y}(R) \rightarrow \infty$ .

There are also circumstances where more general boundary conditions are required:

- In systems where  $R = 0$  is energetically accessible, some states require  $\mathbf{Y}(0) = 0$ .
- In model systems with a Fermi pseudopotential, corresponding to a  $\delta$ -function at the origin or elsewhere, a finite value of  $\mathbf{Y}$  may be required.

MOLSCAT allows the imposition of separate boundary conditions for  $\mathbf{Y}$  in locally closed and open channels at  $R_{\text{min}}$ .

### 1.4. The scattering matrix

The outcome of a collision process is usually described in quantum mechanics by the scattering matrix (S matrix), which contains information on the probability amplitudes and phases for the various possible outcomes. In simple cases (diagonal  $H_{\text{intl}}$  and  $\hat{L}^2$ ), each possible outcome corresponds to one of the channels in the coupled equations. Alternatively, if  $H_{\text{intl}}$  is non-diagonal, each outcome corresponds to an *asymptotic channel* represented by one of the simultaneous eigenvectors of  $H_{\text{intl}}$  and  $\hat{L}^2$  with energy eigenvalue  $E_{\text{intl},i}$ .

Each asymptotic channel  $i$  is *open* if it is energetically accessible as  $R \rightarrow \infty$  ( $E_{\text{intl},i} \leq E$ ) or *closed* if it is energetically forbidden ( $E_{\text{intl},i} > E$ ).

For each  $J_{\text{tot}}$  and symmetry block, solutions to the coupled equations are propagated from deep inside the classically forbidden region at short range to a distance at long range beyond which the interaction potential may be neglected. The wavefunction matrix  $\Psi(R)$  and its radial derivative (or the log-derivative matrix  $\mathbf{Y}(R)$ ) are then matched to the analytic functions that describe the solutions of the Schrödinger equation in the absence of an interaction potential,

$$\Psi(R) = \mathbf{J}(R) + \mathbf{N}(R)\mathbf{K}. \quad (11)$$

where the matrices  $\mathbf{J}(R)$  and  $\mathbf{N}(R)$  are diagonal and are made up of Ricatti-Bessel functions for the open channels and modified spherical Bessel functions for the closed channels. For each channel  $i$ , the Bessel function is of order  $L_i$  and its argument is  $k_i R$ , where  $k_i$  is the asymptotic wavevector such that  $\hbar^2 k_i^2 / 2\mu = |E - E_{\text{intl},i}|$ . For some basis sets,  $L_i$  is non-integer.

The real symmetric  $N \times N$  matrix  $\mathbf{K}$  is then converted to the S matrix,

$$\mathbf{S} = (\mathbf{I} + i\mathbf{K}_{\text{oo}})^{-1}(\mathbf{I} - i\mathbf{K}_{\text{oo}}), \quad (12)$$

where  $\mathbf{K}_{\text{oo}}$  is the open-open portion of  $\mathbf{K}$ .  $\mathbf{S}$  is a complex symmetric unitary matrix of dimension  $N_{\text{open}} \times N_{\text{open}}$ , where  $N_{\text{open}}$  is the number of open channels.

If  $\hat{L}^2$  and  $H_{\text{intl}}$  are both diagonal, the asymptotic channels used for matching to Bessel functions are the same as the channels used to propagate the wavefunction matrix  $\Psi(R)$  or its log-derivative  $\mathbf{Y}(R)$ .

If  $\hat{L}^2$  and/or  $H_{\text{intl}}$  is non-diagonal, MOLSCAT transforms  $\Psi(R)$  or  $\mathbf{Y}(R)$  at  $R = R_{\text{max}}$  into a basis set that diagonalises  $\hat{L}^2$  and  $H_{\text{intl}}$ :

- If  $\hat{L}^2$  is diagonal but  $H_{\text{intl}}$  is not, MOLSCAT constructs the matrix of  $H_{\text{intl}}$  for each value of  $L$  in turn, and diagonalises it. It uses the resulting eigenvectors to transform the corresponding block of  $\Psi(R_{\text{max}})$  or  $\mathbf{Y}(R_{\text{max}})$  into the asymptotic basis set.
- If  $\hat{L}^2$  is non-diagonal (whether  $H_{\text{intl}}$  is diagonal or not), MOLSCAT constructs the complete matrix of  $H_{\text{intl}}$  and diagonalises it. If there are degenerate eigenvalues  $E_{\text{intl},i}$  of  $H_{\text{intl}}$ , it then constructs the matrix of  $\hat{L}^2$  for each degenerate subspace and diagonalises it to obtain eigenvalues  $L_i$  and simultaneous eigenvectors of  $\hat{L}^2$  and  $H_{\text{intl}}$ . It uses the simultaneous eigenvectors to transform  $\Psi(R_{\text{max}})$  or  $\mathbf{Y}(R_{\text{max}})$  into the asymptotic basis set.

Finally MOLSCAT uses the transformed  $\Psi(R_{\text{max}})$  or  $\mathbf{Y}(R_{\text{max}})$ , together with the eigenvalues  $E_{\text{intl},i}$  and  $L_i$ , to extract  $\mathbf{K}$  and  $\mathbf{S}$ .

There are occasional cases where there are sets of vectors that are degenerate or near-degenerate in both  $\hat{L}^2$  and  $H_{\text{intl}}$ . It is possible to define extra operators  $\hat{P}_i$  to aid in resolving such (near-)degeneracies. These extra operators, which need not necessarily contribute to  $H_{\text{intl}}$  or  $\hat{L}^2$ , must nevertheless commute with them. In any (near-)degenerate subspace of the eigenvectors of  $H_{\text{intl}}$  and  $\hat{L}^2$ , MOLSCAT constructs the matrix of the first such operator ( $\hat{P}_1$ ) and finds linear combinations of the degenerate functions that are eigenfunctions of it. If the eigenvalues of  $\hat{P}_1$  are sufficiently non-degenerate, the process ends; if not, it is repeated with operator  $\hat{P}_2$ , and so on.

### 1.5. Cross sections

Experimental observables that describe completed collisions, such as differential and integral cross sections, and scattering lengths, can be written in terms of S-matrix elements. Cross sections typically involve a *partial-wave sum*, with contributions from many values of  $J_{\text{tot}}$ , except at the lowest kinetic energies (in the ultracold regime). By default MOLSCAT uses its S matrices to accumulate degeneracy-averaged state-to-state integral cross sections, which may be written

$$\sigma_{n_i \rightarrow n_f} = \frac{\pi}{g_{n_i} k_{n_i}^2} \sum_{\substack{J_{\text{tot}} \\ M}} (2J_{\text{tot}} + 1) \sum_{\substack{i \in n_i \\ f \in n_f}} \left| \delta_{if} - S_{if}^{J_{\text{tot}}, M} \right|^2. \quad (13)$$

Here  $n_i$  and  $n_f$  label initial and final levels (not states) of the colliding pair,<sup>1</sup> while  $i$  and  $f$  indicate the open channels arising from those levels for total angular momentum  $J_{\text{tot}}$  and symmetry block  $M$ .  $g_{n_i}$  is the degeneracy of level  $n_i$ .

MOLSCAT can calculate line-shape cross sections for the broadening, shifting and mixing of spectroscopic lines for most of the built-in coupling cases. Line-shape cross sections require scattering calculations for the upper and lower states of the spectroscopic transition at the same *kinetic* (not total) energy; if desired, the input energies are interpreted as kinetic energies and the total energies required are generated internally.

MOLSCAT has features to locate scattering resonances, which may produce sharp features in the energy-dependence of cross sections and may also be interpreted as predissociating states of van der Waals complexes. It can calculate the S-matrix eigenphase sum, which is a generalisation of the scattering phase shift to multichannel problems [4], and use it to converge towards a far-off scattering resonance as a function of energy.

MOLSCAT can output S matrices to auxiliary files for later processing. Separate programs are available:

- program DCS [6] to calculate differential cross sections;
- program SBE [7] to calculate generalised transport, relaxation and Senftleben-Beenakker cross sections;
- program RESFIT [8] to fit to eigenphase sums and S-matrix elements to extract resonance positions, widths and partial widths as a function of energy or external field.

### 1.6. Reference energy

By default, the zero of energy used for total energies is the one used for monomer energies, or defined by the monomer Hamiltonians programmed in a plug-in basis-set suite. However, it is sometimes desirable to use a different zero of energy (reference energy). This may be specified:

- as a value given directly in the input file;
- as the energy of a particular scattering threshold or pair of monomer states, which may depend on external fields.

### 1.7. Low-energy collision properties

MOLSCAT has many features designed to facilitate low-energy scattering calculations.

#### 1.7.1. Scattering lengths and volumes

MOLSCAT can calculate scattering lengths or volumes, which may be complex in the presence of inelastic channels. The diagonal S-matrix element in an incoming channel 0 may be written in terms of a complex phase shift  $\eta$ ,

$$S_{00} = \exp(2i\eta). \quad (14)$$

For a channel with low kinetic energy, the phase shift may be expanded in powers of the incoming wavevector  $k$ . The leading term is proportional to  $k$  for  $s$ -wave scattering and  $k^3$  for  $p$ -wave scattering. For higher values of  $L$  the leading power depends on the form of the long-range potential: e.g., for a potential that varies as  $-C_6 R^{-6}$  at long range, the leading term is proportional to  $k^4$  for all  $L > 1$ . MOLSCAT calculates scattering lengths for  $L = 0$  ( $n = 1$ ), volumes for  $L = 1$  ( $n = 3$ ) and hypervolumes for  $L > 1$  ( $n = 4$ ) using the formula [9]

$$a_L(k) = \frac{-\tan \eta}{k^n} = \frac{1}{ik^n} \left( \frac{1 - S_{00}}{1 + S_{00}} \right). \quad (15)$$

It should be emphasised that Eq. 15 is an identity, so that this is a far more general approach than that used by some other programs that take the limit of other (often more complicated) functions as  $k \rightarrow 0$ . The scattering length and volume defined by Eq. 15 become independent of  $k$  at sufficiently low  $k$ .

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<sup>1</sup>For most coupling cases,  $n_i$  and  $n_f$  each represent several quantum numbers, not just one.

### 1.7.2. Characterisation of zero-energy Feshbach resonances

MOLSCAT can converge on and characterise the zero-energy Feshbach resonances that appear in the scattering length as a function of external fields [10]. It can do this for resonances both in elastic scattering, where the scattering length has a simple pole characterised by its position and width and the background scattering length, and in inelastic scattering, where the resonant behaviour is more complex and requires additional parameters [9].

It is often convenient to locate resonances using the associated FIELD program [11] before characterising them with MOLSCAT.

### 1.7.3. Effective range

In the absence of inelastic scattering, the  $s$ -wave scattering length  $a_0$  is real. The near-threshold dependence of the  $s$ -wave scattering phase shift  $\eta$  on kinetic energy  $E_{\text{kin}}$  or wavevector  $k$  is often characterised by an effective-range expansion at small collision momentum

$$k \cot \eta(k) = -\frac{1}{a_0(0)} + \frac{1}{2}r_{\text{eff}}k^2 + \dots \quad (16)$$

Either the scattering length  $a_0(k)$  or its reciprocal can thus be expressed at low energy in terms of the effective range  $r_{\text{eff}}$  [12]. The first of these is numerically unstable near a pole and the second near a zero crossing. MOLSCAT calculates the effective range using both expansions for every energy after the first.

### 1.8. Scattering wavefunctions

If desired, MOLSCAT can calculate the multichannel scattering wavefunction  $\psi(R)$  that is incoming in a single channel and outgoing in all channels, using a generalisation of the method of Hutson and Thornley [13].

### 1.9. Infinite-order sudden approximation

MOLSCAT incorporates code for calculating degeneracy-averaged and line-shape cross sections within the infinite-order sudden (IOS) ansatz. In this formulation, S matrices are calculated from propagations carried out at fixed molecular orientations. The cross sections are written in terms of sums of products of dynamical factors  $Q$  and spectroscopic coefficients  $F$ . The dynamical factors contain all the information about the collision dynamics; they are defined as integrals over the fixed-orientation S matrices, which are evaluated by numerical quadrature. The spectroscopic coefficients contain information about rotor levels and angular momentum coupling. The IOS code has not been used much in recent years, but is retained for backwards compatibility. It does not provide low-energy features such as scattering lengths.

## 2. Systems handled

MOLSCAT can carry out scattering calculations in the close-coupling approximation (with no dynamical approximations except basis-set truncation) for the following pairs of species:

1. Atom + linear rigid rotor [14];
2. Atom + vibrating diatom (rotationally and/or vibrationally inelastic) with interaction potentials independent of diatom rotational state [15];
3. Linear rigid rotor + linear rigid rotor [16, 17, 18];
4. Asymmetric top + linear molecule [19]
5. Atom + symmetric top (also handles near-symmetric tops and linear molecules with vibrational angular momentum) [20, 21];
6. Atom + asymmetric top [20] (also handles spherical tops [22]);
7. Atom + vibrating diatom (rotationally and/or vibrationally inelastic) with interaction potentials dependent on diatom rotational state [23];
8. Atom + rigid corrugated surface: diffractive (elastic) scattering [24, 25]. At present, the code is restricted to centrosymmetric lattices, for which the potential matrices are real.



The close-coupling calculations are all implemented in a fully coupled space-fixed representation, with the calculations performed separately for each total angular momentum and parity.

In addition, MOLSCAT implements a variety of dynamical approximations (decoupling methods) that offer considerable savings of computer time at the expense of accuracy. The methods supported are:

1. Effective potential approximation [26] (seldom used nowadays);
2. Coupled-states (centrifugal sudden) approximation [27];
3. Decoupled  $L$ -dominant approximation [28, 29] (seldom used nowadays).

Not all these approximations are supported for all collision types, though the most common ones are.

In addition to the built-in coupling cases, MOLSCAT provides an interface that allows users to specify sets of coupled equations that arise for different pairs of colliding species. These have been used for numerous different cases, and routines are provided for two cases of current interest:

1. Structureless atom +  $^3\Sigma$  molecule in a magnetic field, demonstrated for  $\text{Mg} + \text{NH}$ ;
2. Two alkali-metal atoms in  $^2\text{S}$  states, including hyperfine coupling, in a magnetic field, demonstrated for  $^{85}\text{Rb}_2$ .

### 3. Propagators

MOLSCAT can solve the coupled equations using a variety of different propagation methods. The propagators currently implemented are:

- Log-derivative propagator of Johnson (LDJ) [30, 31]: This is a very stable propagator. It has largely been superseded by the LDMD propagator.
- Diabatic log-derivative propagator of Manolopoulos (LDMD) [32]: This is a very efficient and stable propagator, especially at short and medium range. It is coded to detect single-channel cases (including IOS cases) automatically and in that case use a more efficient implementation.
- Quasiadiabatic log-derivative propagator of Manolopoulos (LDMA) [33, 34]: This is similar to the LDMD propagator, but operates in a quasiadiabatic basis. It offers better accuracy than LDMD for very strongly coupled problems, but is relatively expensive. It is recommended for production runs only for very strongly coupled problems. However, it is also useful when setting up a new system, because it can output eigenvalues of the interaction matrix at specific distances (adiabats) and nonadiabatic couplings between the adiabatic states.
- Symplectic log-derivative propagators of Manolopoulos and Gray (LDMG) [35]: This offers a choice of 4th-order or 5th-order symplectic propagators. These are 1.5 to 3 times more expensive per step than the LDMD and LDJ propagators, but can have smaller errors for a given step size. They can be the most efficient choice when high precision is required.
- Airy propagator: This is the AIRY log-derivative propagator of Alexander [36] as reformulated by Alexander and Manolopoulos [37]. It uses a quasiadiabatic basis with a linear reference potential (which results in Airy functions as reference solutions). This allows the step size to increase rapidly with separation, so that this propagator is particularly efficient at long range.
- de Vogelaere propagator (DV) [38]: This propagates the wavefunction explicitly, but is much slower than more modern methods, especially for large reduced masses or high scattering energies. It is not recommended except for special purposes.
- R-matrix propagator (RMAT) [39]: This is a stable method that works in a quasiadiabatic basis. It has relatively poor step-size convergence properties, and has largely been superseded by the log-derivative propagators. It is not recommended except for special purposes.

- VIVS propagator: This is the variable-interval variable-step method of Parker *et al.* [40] and is intended for use at long range. It is sometimes very efficient, but the interval size is limited when there are deeply closed channels, so that it is not efficient at long range in such cases. Control of it is considerably more complicated than for other propagators, and it has largely been superseded by the AIRY propagator.
- WKB semiclassical integration using Gauss-Mehler quadrature [41]: This is not a true propagator and can be used only for single-channel problems.

MOLSCAT can use different propagators at short and long range. This is particularly useful for low-energy scattering, where it may be necessary to propagate to very large values of  $R$  to obtain converged results. The AIRY propagator incorporates a variable step size, and can be used to propagate outwards with a fast-increasing step size at long range at very low cost. However, it is not particularly efficient when the interaction potential is fast-varying, so it is often used in combination with a fixed-step-size method such as the LDMD propagator at short and intermediate range.

#### 4. Computer time

The computer time required to solve a set of  $N$  coupled equations is approximately proportional to  $N^3$ . The practical limit on  $N$  is from a few hundred to several thousand, depending on the speed of the computer and the amount of memory available.

The computer time also depends linearly on the number of radial steps required to solve the coupled equations to the desired accuracy. The step size required is typically proportional to the minimum local wavelength, so that the time scales approximately with  $(\mu E_{\max}^{\text{kin}})^{1/2}$ , where  $E_{\max}^{\text{kin}}$  is the maximum local kinetic energy; for scattering calculations,  $E_{\max}^{\text{kin}}$  may be approximated by the sum of the collision energy and the well depth of the interaction potential.

#### 5. Plug-in functionality

##### 5.1. Potential or potential expansion coefficients

The programs internally express the interaction potential as an expansion over the internal coordinates, as in Eq. (7). The expansion coefficients  $v_{\Lambda}(R)$  may be supplied in a variety of ways:

- For very simple potentials, where the functions  $v_{\Lambda}(R)$  are sums of exponentials and inverse powers, the parameters that specify them may be supplied in the input file.
- For more complicated functions, plug-in routines may be supplied to return individual values of  $v_{\Lambda}(R)$  at a value of  $R$  specified in the calling sequence.
- For most of the built-in coupling cases, plug-in routines may be supplied to return the unexpanded potential  $V(R, \xi_{\text{intl}})$  at specified values of  $R$  and the internal coordinates  $\xi_{\text{intl}}$ . The general-purpose potential routine supplied then performs numerical quadrature over  $\xi_{\text{intl}}$  to evaluate the expansion coefficients  $v_{\Lambda}(R)$  internally.
- If none of these approaches is convenient (or efficient enough), a replacement potential routine may be supplied to return the complete potential expansion at once (all values of  $v_{\Lambda}(R)$  at a value of  $R$  specified in the calling sequence).

##### 5.2. Basis sets and coupling matrices

The programs provide an interface for users to supply a set of routines that specify an additional type of basis set, select the elements that will be used in a particular calculation, and calculate the matrices of coupling coefficients for the operators  $\mathcal{V}^{\Lambda}(\xi_{\text{intl}})$  used to expand the interaction potential. The routines must also specify the matrices of  $H_{\text{intl}}$  and  $\hat{L}^2$ , which may be diagonal or non-diagonal. If desired,  $H_{\text{intl}}$  may contain terms that depend on external fields.

### 5.3. External fields and potential scaling

The programs incorporate data structures to handle external electric, magnetic or photon fields. There may be multiple fields at arbitrary relative orientations. Internally, the field-dependent terms in the Hamiltonian are a subset of those in  $H_{\text{intl}}$ ,

$$H_{\text{intl}}(\xi_{\text{intl}}, \mathbf{B}) = \sum_{\Omega} B_{\Omega} \mathcal{H}_{\text{intl}}^{\Omega}(\xi_{\text{intl}}), \quad (17)$$

where the vector  $\mathbf{B}$  represents all the fields present. The elements of  $\mathbf{B}$  may each be expressed as a *nonlinear* function of external field variables (EFVs); the EFVs may thus (for example) represent the magnitudes, orientations, or relative angles of the component fields. MOLSCAT allows calculations on a grid of values of any one EFV, and allows the location and characterisation of low-energy Feshbach resonances as a function of one EFV with all the others fixed.

The programs also allow calculations as a function of a scaling factor that multiplies the entire interaction potential, or a subset of the potential expansion coefficients  $v_{\Lambda}(R)$ . The scaling factor is handled internally using the same structures as external fields.

## 6. Distributed files and example calculations

### 6.1. Distributed files

The program is supplied as a tarred zipped file, which contains:

- the full program documentation in pdf format;
- a directory `source_code` containing
  - the Fortran source code;
  - a GNU makefile (`GNUmakefile`) that can build the executables needed for the example calculations;
- a directory `examples` containing
  - a sub-directory `input` containing input files for the example calculations described below;
  - a sub-directory `output` containing the corresponding output files;
- a directory `data` containing auxiliary data files for some potential routines used in the example calculations;
- a plain-text file `README` that gives information on changes that may be needed to adapt the GNUmakefile to a specific target computer.
- a plain-text file `COPYING` that contains the text of the GNU General Public License, Version 3.

### 6.2. Example calculations

The executables used for different calculations may differ in the routines linked to construct the basis set, specify the internal Hamiltonian, and evaluate the interaction potential. The executables required for the example calculations can all be built using `GNUmakefile`.

#### 6.2.1. All available propagators

input file: `molscat-all_propagators.input`  
 executable: `molscat-basic`

`molscat-all_propagators.input` performs close-coupling calculations for a single partial wave and parity for a simple model of collisions between an atom and a linear rigid rotor and prints the resulting S matrix. The radial potential coefficients are provided in the input file and consist of a Lennard-Jones 12-6 potential for  $\lambda = 0$  and a dispersion-like  $R^{-6}$  form for  $\lambda = 2$ . The calculation is repeated using combinations of short-range and long-range propagators that exercise every propagation method available in MOLSCAT (though not every possible combination).

#### 6.2.2. All available decoupling approximations

input file: `molscat-all_iadds.input`  
executable: `molscat-basic`

`molscat-all_iadds.input` contains input data for a similar model system, extended this time to include vibrations of the linear rotor. The radial potential coefficients are again provided in the input file, and all consist of inverse-power functions of  $R$ . The LDMD/AIRY hybrid propagation scheme is used. MOLSCAT first performs close-coupling calculations and then repeats the calculation using every decoupling approximation available.

#### 6.2.3. Location of quasibound state (Feshbach resonance) for $\text{Ar} + \text{HF}$

input file: `molscat-Ar_HF.input`  
executable: `molscat-Rg_HX`  
also required: `data/h2even.dat`

`molscat-Ar_HF.input` demonstrates the procedure for locating a narrow resonance in the S-matrix eigenphase sum as a function of energy. It performs calculations on the  $\text{H}_6(4,3,2)$  potential of Hutson [42] for the ground ( $v = 0$ ) vibrational state of HF, using the LDMD propagator. It first does scattering calculations at 5 energies reasonably close to the resonance (but actually over 1000 widths away) and uses the resulting eigenphase sums to estimate the resonance position. It then does another 5 calculations around the estimated resonance position, and this time finds that they span the resonance (which is between points 2 and 3 of the second set of 5). The formula used for estimating resonance positions is valid only far from resonance, so it reports that the second set of points cannot safely be used to locate the resonance energy.

The extrapolation procedure used in this example amplifies any tiny differences between computers due to finite-precision arithmetic. The second set of 5 energies is commonly significantly different on different computers; this does not indicate an error.

#### 6.2.4. Line-shape cross sections for $\text{Ar} + \text{CO}_2$

input file: `molscat-Ar_CO2.input`  
executable: `molscat-Rg_CO2`

`molscat-Ar_CO2.input` performs close-coupling calculations of line-shape cross sections for the S(10) Raman line of  $\text{CO}_2$  in Ar, using the single repulsion potential of Hutson *et al.* [43] with the LDMD propagator at short range and the AIRY propagator at long range. The calculations are at a kinetic energy of  $200 \text{ cm}^{-1}$  and the total energies are calculated internally. The program prints cross sections accumulated up to the current value of  $J_{\text{TOT}}$ ; the convergence of the partial-wave sum may be compared with Fig. 2 of ref. [44].

#### 6.2.5. Line-shape cross sections for $\text{Ar} + \text{H}_2$

input file: `molscat-Ar_H2.input`  
executable: `molscat-Rg_H2`  
also required: `data/h2even.dat`

`molscat-Ar_H2.input` calculates pure rotational Raman line widths and shifts across a shape resonance at a collision energy near  $14 \text{ cm}^{-1}$ . It uses the  $\text{BC}_3(6,8)$  interaction potential of Carley and Le Roy [45], evaluated for  $\text{H}_2$  states  $(j, v) = (0, 0)$ ,  $(2, 0)$  and  $(4, 0)$  using  $\text{H}_2$  matrix elements in the file `data/h2even.dat`. The line-shape calculations require S matrices evaluated at the same *kinetic* energy for different rotational states of  $\text{H}_2$ ; the program treats the input energies as kinetic energies and generates the total energies required. The results may be compared with Figure 2(a) of ref. [23].

#### 6.2.6. Cross sections for rigid rotor + rigid rotor collisions

input file: `molscat-ityp3.input`  
executable: `molscat-H2_H2`

`molscat-ityp3.input` contains input data for collisions between para- $\text{H}_2$  and ortho- $\text{H}_2$ . The interaction potential is that of Zarur and Rabitz [46].

MOLSCAT calculates elastic and state-to-state inelastic cross sections. This calculation requires that contributions from partial waves are accumulated until the partial-wave sums are converged within the

limits set by the input data. Two pairs of calculations are performed, first with close-coupling calculations and then with the coupled-states approximation. All calculations use the LDMD/AIRY hybrid propagation scheme.

Each calculation is done twice; one in which the radial potential coefficients are provided, and one in which the unexpanded potential is provided and is expanded by quadrature by the program. The two calculations illustrate the equivalence of the two methods.

#### 6.2.7. Cross sections for atom + symmetric top collisions, with automated testing of propagator convergence

input file: `molscat-ityp5.input`  
 executable: `molscat-basic`

`molscat-ityp5.input` contains input data for atom + symmetric top collisions between He and ortho-NH<sub>3</sub>, taking account of the tunnelling splitting of NH<sub>3</sub>. It uses a simple analytical interaction potential and the hybrid propagation scheme. The input file uses `ISYM(3) = 1` to select rotational functions of E symmetry and `ISYM(4) = 1` to specify that the H nuclei are fermions. The first four calculations are for a single partial wave and exercise the convergence-testing code in MOLSCAT, testing the convergence with respect to step size (chosen in two ways), and with respect to the start point and end point of the propagation. The final two calculations carry out full cross-section calculations, using converged values for the propagation variables, first with close-coupling calculations and then with the coupled-states approximation.

#### 6.2.8. Cross sections for atom + spherical top collisions

input file: `molscat-ityp6.input`  
 executable: `molscat-Ar_CH4`

`molscat-ityp6.input` contains input data for atom + spherical top collisions between Ar and CH<sub>4</sub>, using the interaction potential of Buck *et al.* [47]. The ground-state rotational constants and the tetrahedral centrifugal distortion constant  $d_t$  are specified in the input file and the program uses them to calculate properly symmetrised spherical-top wavefunctions. The input file selects CH<sub>4</sub> rotor functions of A symmetry by setting `ISYM` to 224. The cross sections use the automatic total angular momentum option `JTOTU = 99999` with a convergence tolerance (`OTOL`) of 0.0001 to give well-converged inelastic cross sections, but the diagonal convergence tolerance `DTOL` is set to 10.0 so that the partial-wave sum terminates before the elastic cross sections are converged. The results may be compared with Table VI of ref. [48], although they do not agree exactly because the results in the paper are averaged over the experimental distribution of collision energies.

#### 6.2.9. Atom-surface scattering

input file: `molscat-ityp8.input`  
 executable: `molscat-basic`

`molscat-ityp8.input` contains input data for diffractive scattering (`ITYPE = 8`) of He from solid LiF, using the model potential of Wolken [24]. It uses the LDMD propagator at two energies.

#### 6.2.10. Cross sections for Mg + NH in a magnetic field

input file: `molscat-Mg_NH.input`  
 executable: `molscat-Mg_NH`  
 also required: `data/pot-Mg_NH.data`

`molscat-Mg_NH.input` contains input data for cold collisions of NH with Mg in a magnetic field. It uses a plug-in basis-set suite for a <sup>3</sup>Σ diatom colliding with a structureless atom. Radial potential coefficients are obtained by RKHS interpolation using the interaction potential of Soldán *et al.* [49]. The coupled equations are solved using the LDMD/AIRY hybrid propagation scheme.

The basis-set suite implements two different forms of the monomer Hamiltonian, including and excluding the off-diagonal matrix elements of the spin-spin operator. The input file specifies runs with both of these. The approximation does not actually produce any saving in computer time in this case.

The input file requests calculations at kinetic energies of 1, 10 and 100 mK above the  $n = 0$ ,  $j = 1$ ,  $m_j = 1$  threshold of NH.

These calculations are similar to (a subset of) those of Wallis *et al.* [50], although the test run uses a smaller basis set than ref. [50]. Convergence at 100 mK requires inclusion of incoming partial waves up to  $L = 3$ , which requires values of  $M_{\text{tot}}$  from  $-2$  to  $4$  for incoming  $m_j = 1$ .

MOLSCAT can accumulate cross sections from calculations for different values of  $M_{\text{tot}}$  and parity at a single field. The first part of the test run, including the off-diagonal matrix elements of the spin-spin operator, illustrates the scheme used for identification of levels for systems with non-diagonal Hamiltonians, where not all threshold channels may be known at the point where the first partial cross sections are calculated.

#### 6.2.11. Characterisation of magnetically tunable Feshbach resonances and calculation of effective range for $^{85}\text{Rb} + ^{85}\text{Rb}$

input file: `molscat-Rb2.input`

executable: `molscat-Rb2`

`molscat-Rb2.input` contains input data for low-energy  $^{85}\text{Rb} + ^{85}\text{Rb}$  collisions in a magnetic field, using a plug-in basis-set suite for a pair of alkali-metal atoms in a magnetic field, including hyperfine interactions. It uses the potential of Strauss *et al.* [51], implemented with potential coefficients incorporated in the executable. All the calculations use the LDMD/AIRY hybrid propagation scheme.

This test run characterises 4 different low-energy Feshbach resonances as a function of magnetic field, using the characterisation algorithms described by Frye and Hutson [10]. The first resonance is in purely elastic scattering in the lowest (aa) scattering channel, so produces a pole in the scattering length as a function of magnetic field. The second and third resonances occur in collisions at excited thresholds, where weak inelastic scattering is possible and the pole is replaced by an oscillation [9]. The fourth is subject to strong background inelasticity. Following those 4 calculations, a further calculation obtains the effective range across the strong resonance observed in the aa channel near 850 G, from scans across the resonance at energies of 100 and 200 nK.

The basis-set suite for this interaction requires information about the hyperfine properties of the atoms in an additional namelist block named `&BASIS9`. The potential expansion comprises 3 terms: the singlet and triplet interaction potentials, and the spin-spin dipolar term, which is modelled in the form

$$\lambda(R) = E_h \alpha^2 \left[ \frac{g_S^2}{4(R/a_0)^3} + A \exp(-\beta R/a_0) \right]. \quad (18)$$

## 7. Program history

The MOLSCAT program was originally written by Sheldon Green in the 1970s, incorporating propagators from several different authors and adapting them to share the same input / output structures and mechanisms for generating matrix elements of the molecular Hamiltonian and interaction potential. Early versions of the program handled atom-molecule and molecule-molecule scattering, with a variety of additional coupling cases added between versions 1 (1973) and 7 (1979) [52]. Both full space-fixed close-coupling calculations and decoupling approximations such as coupled states / centrifugal-sudden (CS), infinite-order sudden (IOS) and decoupled  $L$ -dominant (DLD) approximations were implemented. The program calculated integral elastic, state-to-state inelastic and line-shape cross sections internally and wrote S matrices to a file that could be used for post-processors, including DCS [6] for differential cross sections and SBE [7] for cross sections associated with transport and relaxation properties and Senftleben-Beenakker effects.

Jeremy Hutson became a co-author of MOLSCAT in 1982 and collaborated with Sheldon Green on its development until Green's death in 1995. Major changes in this period included new coupling cases, including the diffractive scattering of atoms from crystal surfaces, the replacement of some older propagators with new ones, and code to handle scattering resonances (with post-processor RESFIT [8] for fitting resonance parameters). In addition, an interface was added in version 11 (1992) to allow the inclusion of plug-in coupling cases with angular momentum algebra and/or interaction potential expansions that were not already present in the code.

The last version of MOLSCAT produced by Green and Hutson in collaboration was version 14 in 1994. This was distributed via the CCP6 collaboration in the UK [53] and via the NASA GISS website. Version 14 formed the basis of a parallel version named PMP MOLSCAT, produced by George McBane [54].

There has been no fully documented publication of the program since MOLSCAT version 14.

### 7.1. Principal changes in version 2019.0

- The basis-set plug-in mechanism has been extended to allow propagation in basis sets that are not eigenfunctions of the internal Hamiltonian  $H_{\text{intl}}$  and/or  $\hat{L}^2$ . This makes implementing new types of system much simpler than before, especially where the individual interaction partners have complicated Hamiltonians.
- If  $H_{\text{intl}}$  or  $\hat{L}^2$  is non-diagonal, the propagated wavefunction or log-derivative matrix is transformed into a basis set that is diagonal in both operators before matching to long-range functions to extract the S matrix.
- The basis-set plug-in functionality has been used to add new capabilities to carry out calculations in external fields (electric, magnetic, and/or photon) and to loop over (sets of) values of the fields.
- The S matrix is now processed to calculate scattering lengths (or volumes or hypervolumes)  $a_L$  [actually  $k$ -dependent complex scattering lengths or volumes  $a_L(k)$ ] for any low-energy scattering channels. MOLSCAT can also extrapolate the real part of  $a_0(k)$  to  $k = 0$  and calculate the effective range  $r_{\text{eff}}$ .
- MOLSCAT can now converge on and characterise Feshbach resonances as a function of external field. This is implemented for both the elastic case, where resonances appear as poles in the scattering length/volume, and the inelastic case, where the resulting decayed resonances have more complicated signatures.
- MOLSCAT can now calculate a multichannel scattering wavefunction that is incoming in a single channel and outgoing in all open channels.
- A more general mechanism for combining propagators for use at short and long range has been implemented, which allows any sensible combination.
- A more general choice of log-derivative boundary conditions at the starting point for propagation is now allowed.
- An additional propagation approach [35] has been included, implemented by George McBane, which takes advantage of the symplectic nature of the multi-channel radial Schrödinger equation.

## 8. Acknowledgements

We are grateful to an enormous number of people who have contributed routines, ideas, and comments over the years. Any attempt to list them is bound to be incomplete. Many of the early contributors are mentioned in the program history in section 7. In particular, we owe an enormous debt to the late Sheldon Green, who developed the original MOLSCAT program and established many structures that have proved general enough to support the numerous later developments. He also developed the DCS and SBE post-processors. Robert Johnson, David Manolopoulos, Millard Alexander, Gregory Parker and George McBane all contributed propagation methods and routines. Christopher Ashton added code to calculate eigenphase sums and developed the RESFIT post-processor. Timothy Phillips developed code for interactions between asymmetric tops and linear molecules. Alice Thornley developed methods to calculate bound-state wavefunctions from log-derivative propagators and George McBane extended them to scattering wavefunctions. Maykel Leonardo González-Martínez worked on the addition of structures for non-diagonal Hamiltonians, including magnetic fields, and Matthew Frye contributed algorithms for converging on low-energy Feshbach resonances (both elastic and inelastic).

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